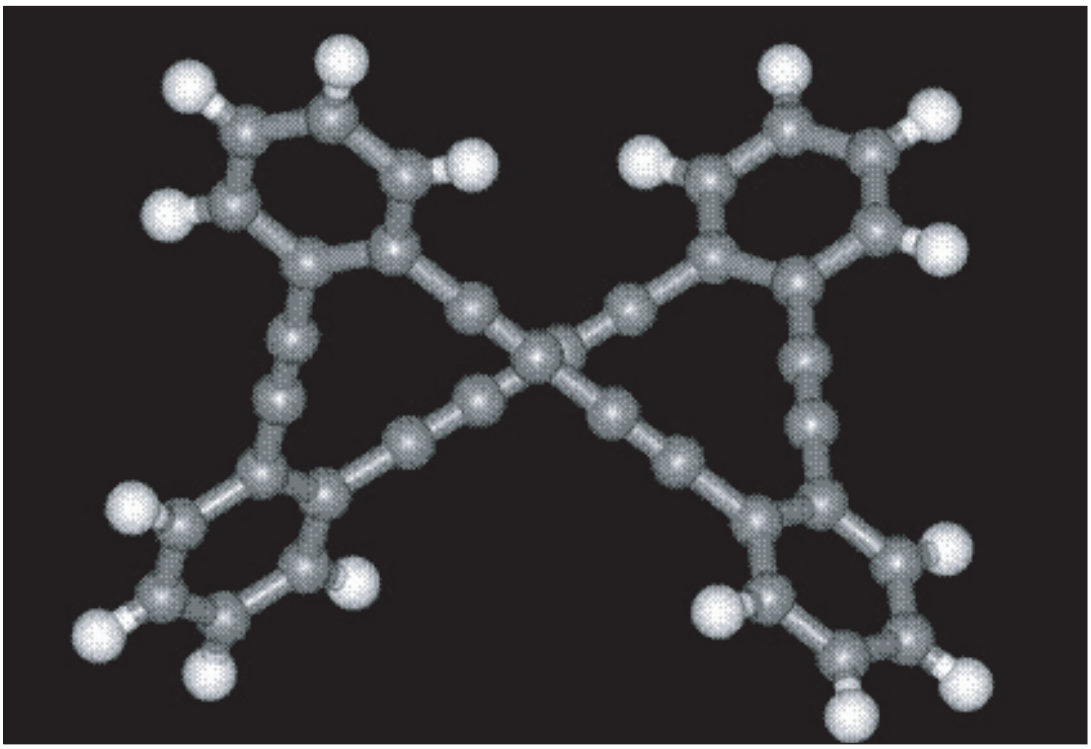
Air Force Research Laboratory|AFRL
Science and Technology for Tomorrow's Air and Space Force

Success Story

HIGH-ENERGY MOLECULE MORPHING



Imagine the capability to simulate complex chemical formulations that will enable national defense and space adventures. Unlike the popular simulation games that are available to the general public, advanced computer capabilities enable dedicated researchers to determine the potential of future rocket fuel ingredients and even provide research chemists a pathway to their safe formulation. Researchers use advanced computational methods to model and predict several key properties of unknown chemical compounds. These methods include calculations of the electronic and molecular structures, heats of formation, vibrational spectra, and nuclear magnetic resonance chemical shifts. Reaction pathways for synthesis, combustion, and decomposition are also computed.

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Accomplishment

Using computational chemistry software on supercomputers located at the Department of Defense (DoD) Major Shared Resource Centers (MSRC), the AFRL Propulsion Directorate's High-Energy-Density Matter program's theoretical chemistry researcher, Dr. Jerry Boatz, can identify new compounds at the molecular level and predict many of their properties that can be measured in the laboratory. This helps identify powerful additives or formulas that can unleash enormous energy for rocket propulsion. Researchers use these calculations to identify the most promising chemical candidates and to guide experimental efforts in synthesis and characterization.

One of the most important recent results of this scientific approach was the identification and successful synthesis of the first high-energy and stable polynitrogen ion species in more than a century. Until 1998, only two all-nitrogen species had ever been isolated in bulk quantities, but calculations showed that other polynitrogens might exist.

Background

Researchers from the DoD, AFRL, academia, and industry use high-performance computers to assist in solving complex technical problems. AFRL's laboratory at Edwards Research Site uses DoD MSRC supercomputers to help design new rocket propellant ingredients for AFRL. There are four MSRCs within the DoD, each containing some of the world's most powerful computers. One of them, an IBM pSeries 690 Turbo system with over 1,400 processors (located at the Naval Oceanographic Office MSRC), is the 18th-largest computer in the world and has a peak computational speed of 6.1 trillion floating-point operations per second.

Propulsion
Emerging Technologies

Additional Information

To receive more information about this or other activities in the Air Force Research Laboratory, contact TECH CONNECT, AFRL/XPTC, (800) 203-6451 and you will be directed to the appropriate laboratory expert. (04-PR-33)